Hierarchically Informed Engineering Models For Predictive Modeling of Turbulent Premixed Flame Propagation in Pre-chamber Turbulent Jet Ignition

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DOE program managers — Michael R. Weismiller, Walter G. Parker

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Project ID: ACE151

Overview

Timeline

Start	Jan 1, 2020
End	Dec 31, 2022
Budget period 1	Jan 1-Dec 31, 2020
Complete	~50% of budget period 1

Budget

Total Award	$1,093,781
Purdue	$650,000
Argonne (FFRDC)	$225,000
Cost share (20% from Purdue)	$218,781
Budget period 1	$386,827

Barriers

- "Understanding and robust modeling tools for rapidly screening proposed designs based on sound metrics are lacking"
- "More robust ignition systems for lean and EGR, as well as boosted conditions that reduce combustion variability are needed"

— U.S. DRIVE roadmaps

- This work overcomes these barriers by developing accurate and efficient models for turbulent flame propagation initiated by a pre-chamber turbulent jet ignition source.

Partners

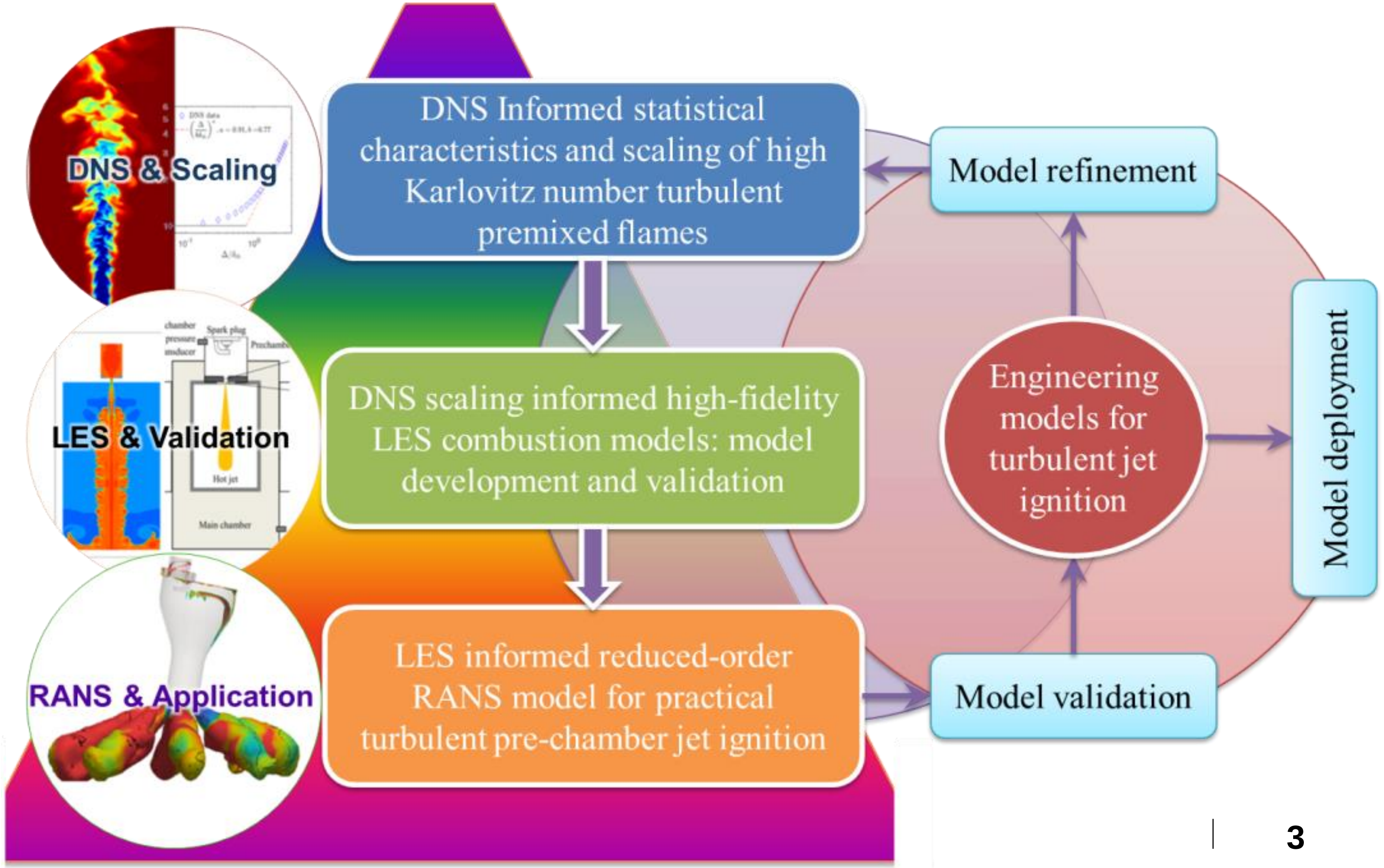
- Sandia National Laboratory
- Purdue University
- Argonne National Laboratory

Relevance

Project Goal

Significantly improve the predictive accuracy and efficiency of turbulent combustion sub-models for the simulations of premixed flame propagation initiated by pre-chamber turbulent jet ignition.

- Objective 1: Acquire statistical properties of high-Karlovitz turbulent premixed flames from direct numerical simulations (DNS) to provide theoretical basis for pre-chamber turbulent jet ignition (TJI) model;
- Objective 2: Develop high-fidelity large-eddy simulation (LES) model for TJI to yield consistency with the acquired statistical properties from DNS;
- Objective 3: Develop engineering Reynolds-averaged Navier-Stokes (RANS) model for TJI through machine learning by using data from high-fidelity LES.



A hierarchically informed engineering model for turbulent flame propagation

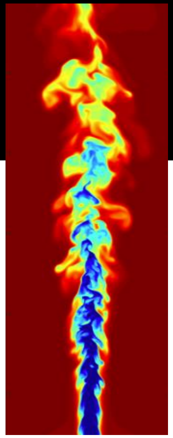
Milestones

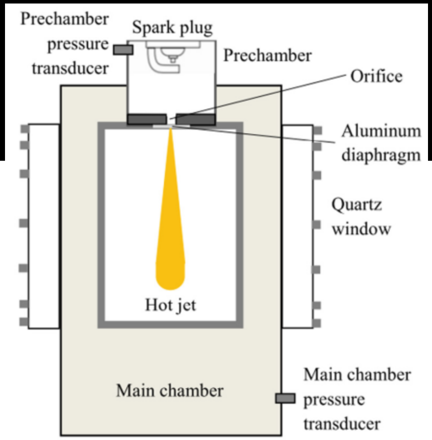
budget period 1, Jan 1-Dec 31, 2020

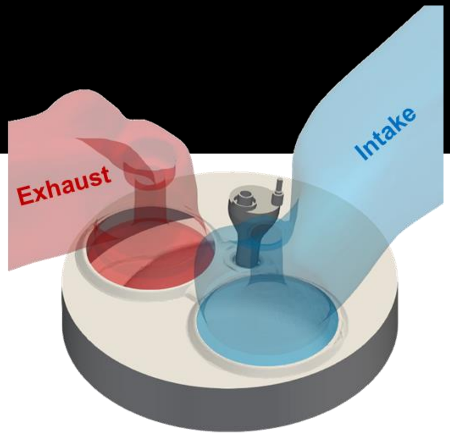
Milestone	Type	Description	Schedule	Status
Hypothesis testing of power-law scaling in high-Karlovitz turbulent flames is complete	Technical	Hypothesis testing of the existence of power-law scaling of sub-filter scaling mixing in high-Karlovitz turbulent jet flames has been completed from both global and local perspectives.	Q1	Completed
Parametric and sensitivity analysis of the power-law scaling is complete	Technical	The parametric analysis of the dependence of the power-law scaling has been completed on flow, turbulence, and thermochemical properties. The sensitivity of the power-law scaling has also been quantified.	Q2-Q3	On-Schedule
A priori testing of the mixing frequency model is complete	Technical	*A priori* testing of the mixing frequency model that can be used for LES modeling has been finished which is based on the power-law scaling verified above.	Q3-Q4	On-Schedule
Statistical power-law scaling has been verified in high-Karlotivz turbulent premixed flames.	Go/No Go	Verification of power-law scaling of sub-filter scale mixing in high-Karlotivz turbulent premixed flame propagation has been achieved to show universal behavior of mixing, paving a theoretical foundation for the predictive LES model development for TJI.	End of Q4	On-Schedule

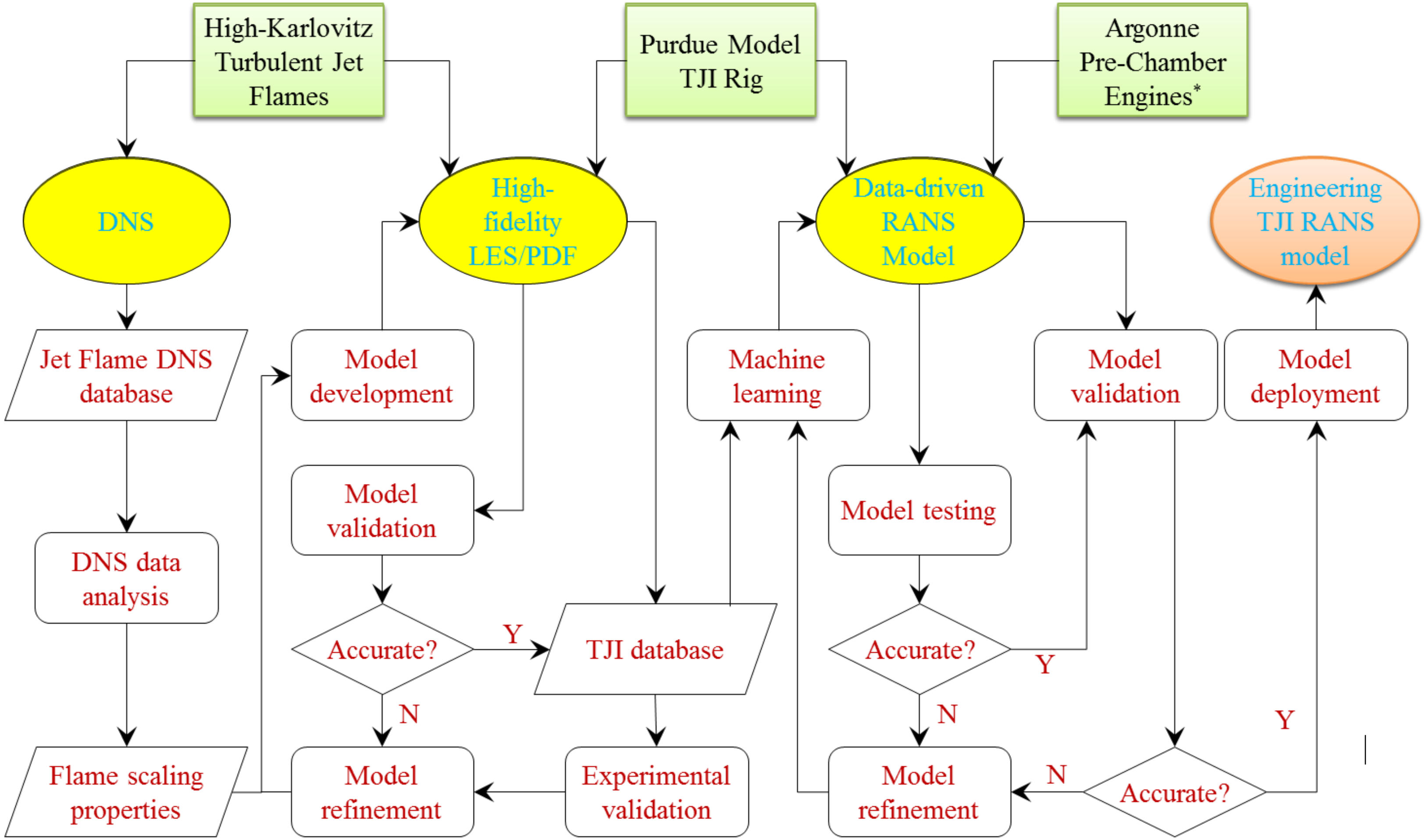
Approach

- **Three levels of model descriptions**
  - Direct Numerical Simulations (DNS)
  - Large-eddy simulations and probability density function (LES/PDF)
  - Reynolds-averaged Navier-Stokes (RANS)
- **Three levels of testing complexities**
  - Sandia premixed jet flame DNS case
  - Purdue model TJI rig
  - Argonne MD single cylinder engine with TJI
- **One model target**
  - Engineering TJI RANS model





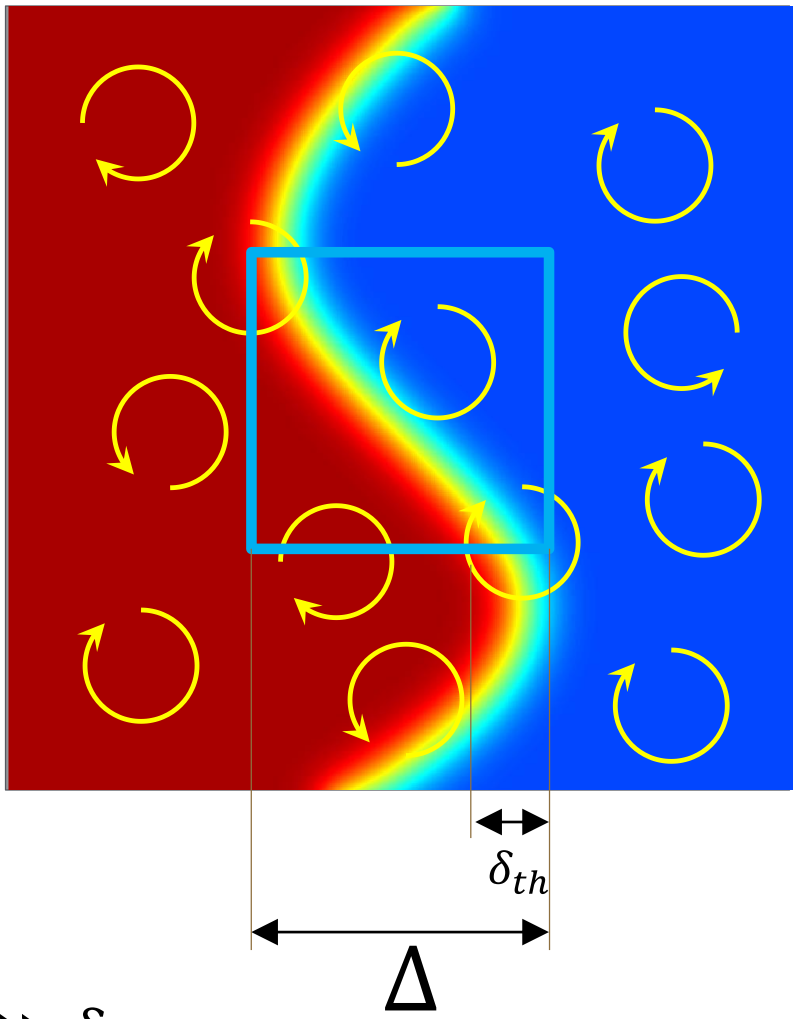




Modeling turbulent premixed combustion

- **Modeling challenges**
  - LES/PDF approach
  - Mixing model bottleneck

- **How to model mixing?**
  - Without a flame, determined by
    - ✓turbulent transport (Γ_t)
    - ✓turbulence resolution scale (Δ)
  - With a flame, determined by
    - ✓turbulent transport (Γ_t)
    - ✓Flame thermal thickness (δ_{th})
    - ✓Different scalars



$$\Omega \sim \frac{\Gamma_t}{\Delta^2}$$

$$\Omega \sim \frac{\Gamma_t}{\delta_{th}^2}$$

$$\Omega \sim \frac{\Gamma_t}{\Delta^2} \times F$$

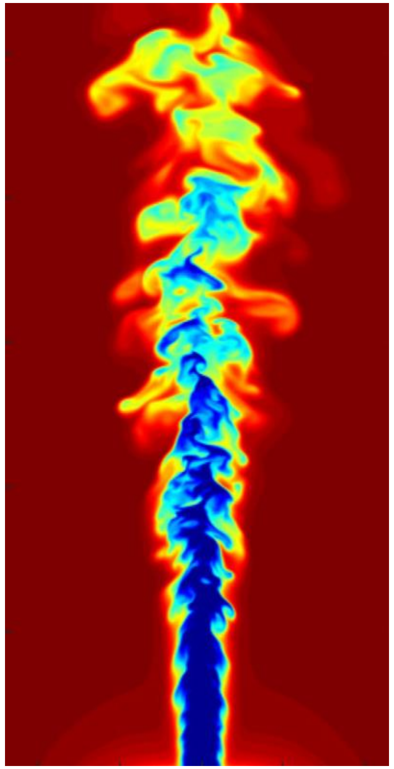
$$F \sim \begin{cases} \left(\dfrac{\Delta}{\delta_{th}}\right)^2 & \text{if } \Delta \gg \delta_{th} \\ 1 & \text{otherwise} \end{cases}$$

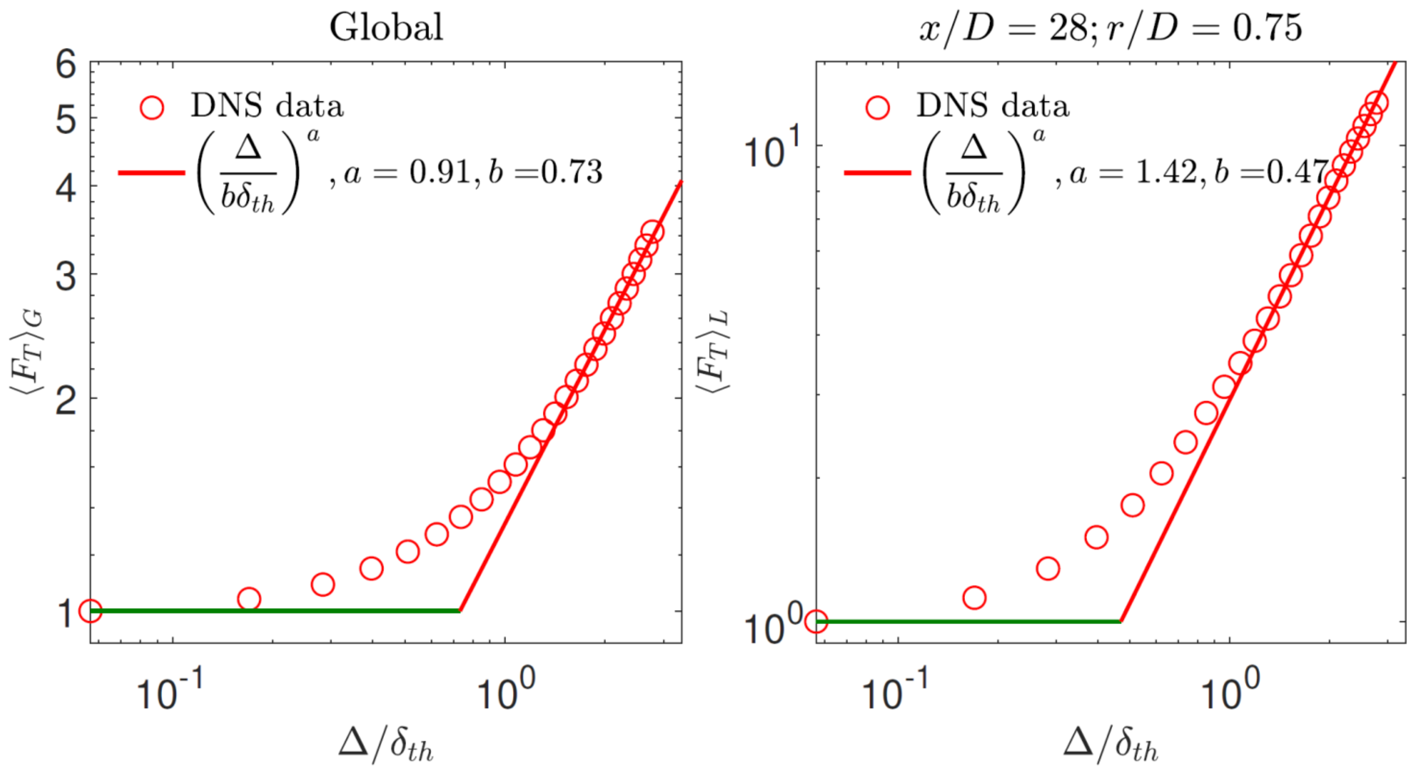
- **Hypothesis**

$$F \sim \left(\frac{\Delta}{\delta_{th}}\right)^a \quad \text{if } \Delta \gg \delta_{th}$$

Technical Accomplishments and Progress

Hypothesis testing





- Multiple scalars
  - Temperature
  - Species
- DNS informed model

$$F = 1 + \left(\frac{\Delta}{b\delta_{th}}\right)^a$$

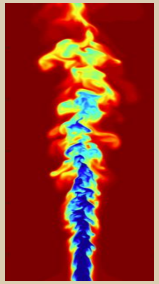
$$a = \mathrm{Const}$$

$$b = f(\mathrm{Re}, \mathrm{Ka})$$

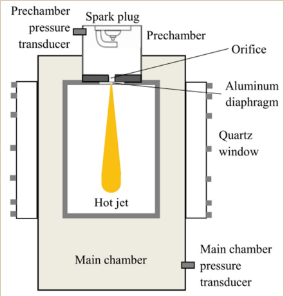
- The power law scaling is broadly observed at different locations for different scalars
- An DNS informed model for mixing has been formulated
- It paves a solid theoretical foundation for a predictive study of TJI

Collaboration and Coordination with other Institutions

Sandia National Lab (J.H. Chen)
Zhejiang University (H. Wang)
University of New South Wales (E.R. Hawkes)

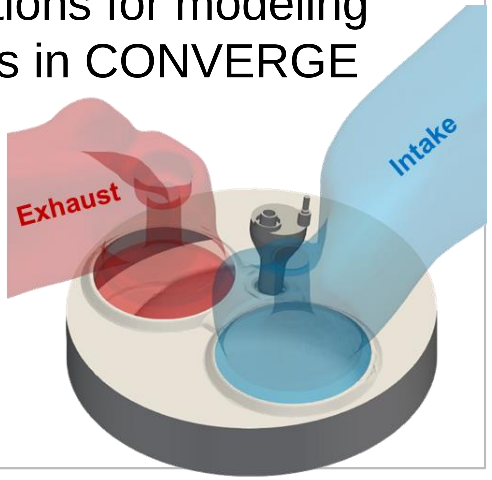


Purdue University (L. Qiao)



Argonne National Lab (R. Scarcelli)

- Supply experimental validation data for the Argonne MD engine
- Conduct model validation
- Work done or being conducted
  - Identifided test conditions for modeling
  - Setting up simulations in CONVERGE CFD



		Unfueled PCSI		Fueled PCSI	
Engine speed	rpm	1200			
Intake boost pressure	bar	1.16		1.04	
Exhaust back pressure	bar	0.98		0.98	
Spark ignition timing	CAD aTDCf	-17		-17.5	
Excess-air ratio (λ_{intake})	-	**1.50**	**1.65**	**1.91**	**2.24**
Fuel ratio of PC/Intake	%	-	-	2.2, 4.1, 6.6	**7.7**
Engine load (nIMEP)	bar	8.1	7.6	5.4, 5.5, 5.7	4.7

Pick one of the two

Pick one of the three

Engine data: courtesy of A. Shah and M. Biruduganti, ANL

Proposed Future Research

Follow the project plan in Budget Periods 1 and 2

- Development of a power-law scaling model for the mixing in premixed combustion.
- Validation of the power-law scaling mixing model in Sandia DNS jet flame.
- Development of regime adaptive models for TJI with multi-regime combustion.

PURDUE UNIVERSITY

- Setup of simulations for the identified engine testing conditions including model geometry and meshing.
- Simulations of the Argonne engine with conventional combustion models to verify the model validation framework

Argonne NATIONAL LABORATORY

Any proposed future work is subject to change based on funding levels.

SUMMARY

- The goal of project is to improve the predictive accuracy and efficiency of turbulent combustion sub-models for the simulations of premixed flame propagation initiated by pre-chamber turbulent jet ignition.
- A hierarchical approach is developed to deduce accurate and efficient engineering models for TJI.
- A power-law scaling for the rate of mixing has been established based on DNS, which paves a solid theoretical foundation to support the proposed hierarchical approach.
- The project team is making steady and planed progress towards the milestones.

Technical Backup Slides

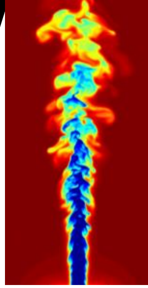
[redacted]

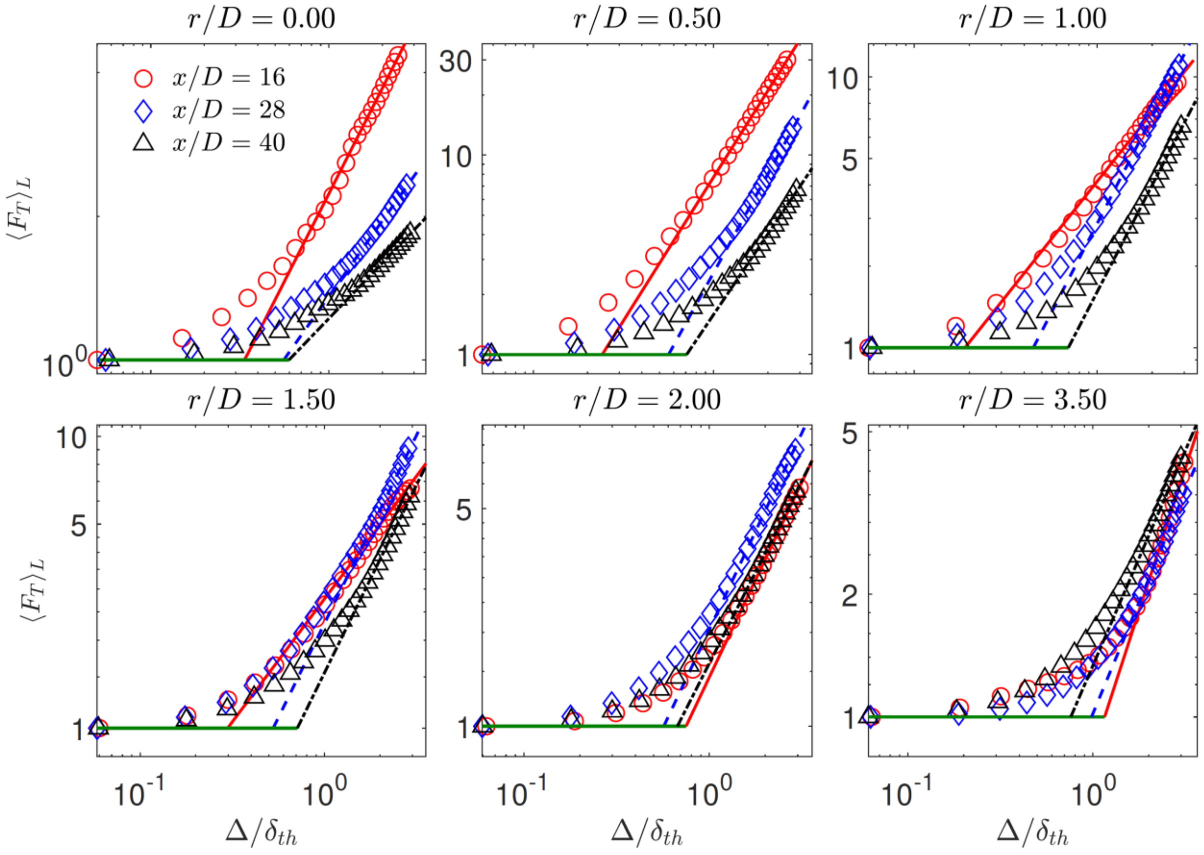
Milestones

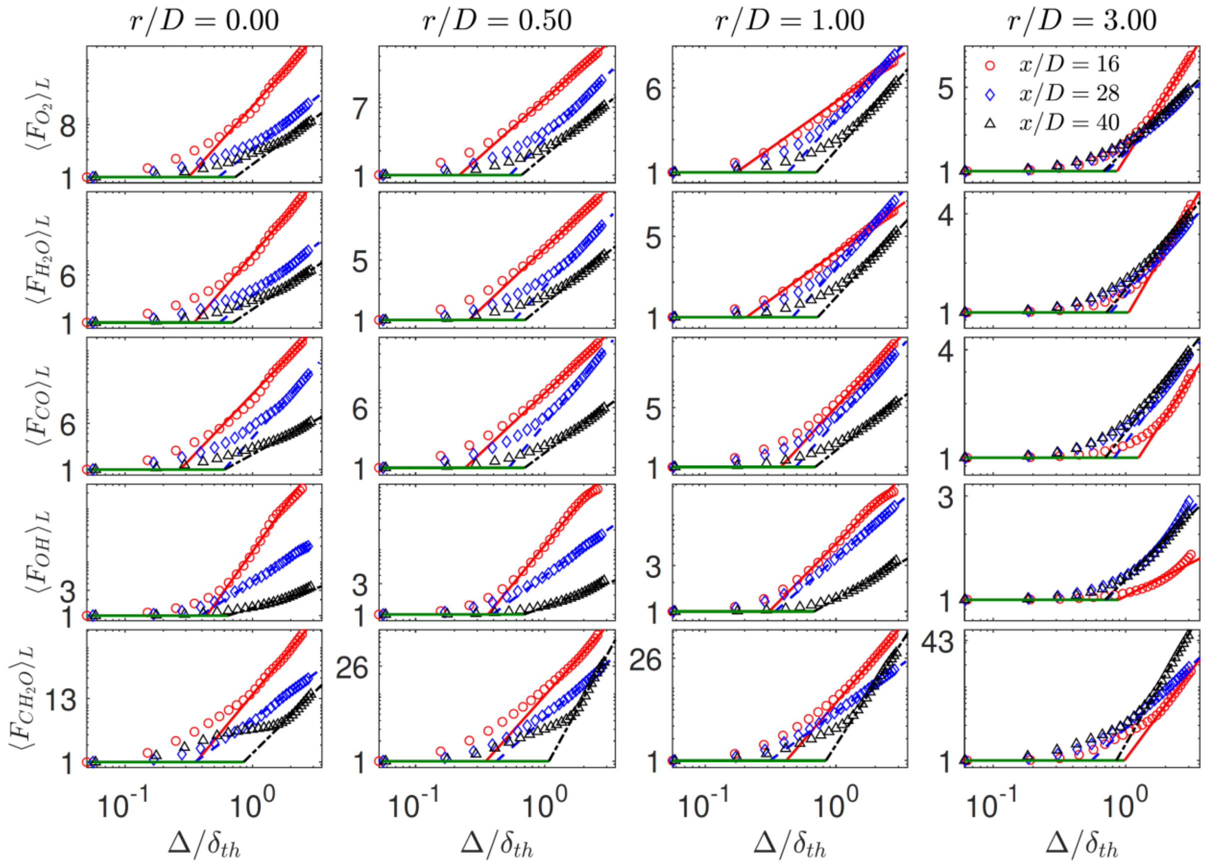
budget period 2, Jan 1-Dec 31, 2021

Milestone	Type	Description
A posteriori testing of the mixing frequency model is complete	Technical Q1	The mixing frequency model informed by the power-law scaling observed in DNS has been incorporated in actual LES and *a posteriori* testing of the model has been completed to further validate the accuracy of the model.
Development and validation of a multi-regime model for TJI is complete	Technical Q2	The development of regime-adaptive LES model to capture multi-regime combustion in TJI systems has been completed, including the model validation in a transient jet flame test case exhibiting bi-modal and multi-regime combustion.
Validation of the developed high-fidelity LES model for TJI in Purdue model TJI rig is complete	Technical Q3-Q4	The model components based on the power-law scaling and multi-regime combustion model have been integrated together and the model validation in the Purdue model TJI rig has been finished.
A high-fidelity LES combustion model for TJI has been developed and validated	Go/No Go	A targeted high-fidelity predictive LES combustion model for TJI has been achieved to provide a tool for the reduced-order model development afterward. The model has been validated against the Purdue model TJI rig to reproduce the measured characteristics of the TJI rig including but not limited to the pressure rising history in pre-chamber and main chamber and the ignition timing. An overall error of the model prediction relative to the measurements within 30% is targeted.

Technical Accomplishments and Progress

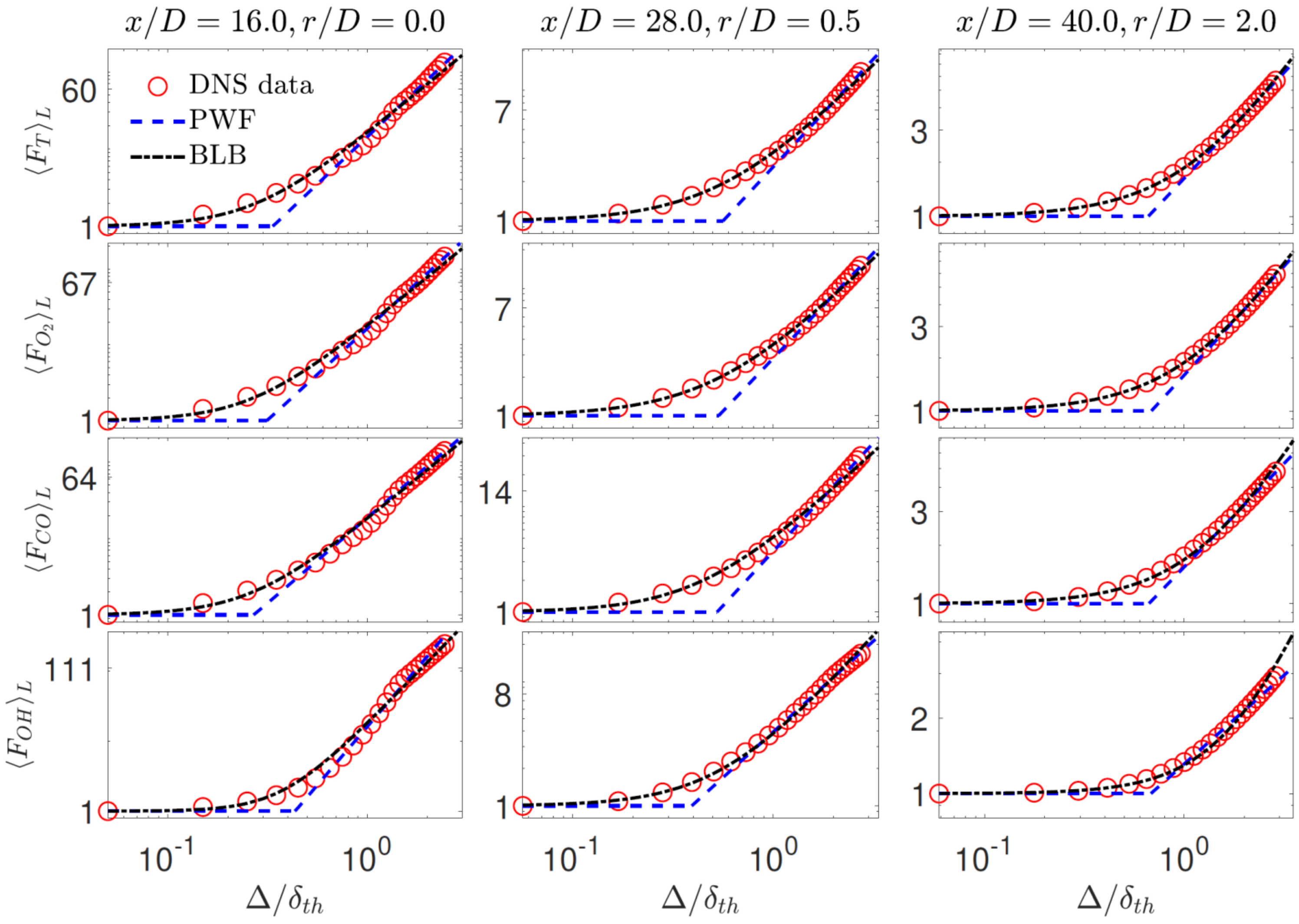


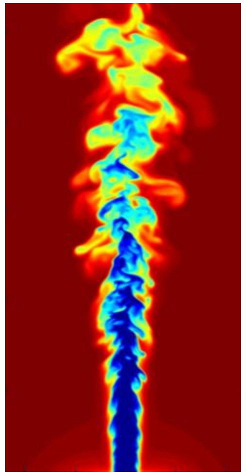




- The power law scaling is broadly observed at different locations for different scalars in the Sandia DNS jet flame

Technical Accomplishments and Progress





$$F = 1 + \left(\frac{\Delta}{b\delta_{th}}\right)^a$$

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- A blending model for F and its examination and validation in the Sandia DNS jet flame

Collaboration and Coordination with other Institutions

Argonne Engine Test Facility

- Single Cylinder Engine setup (Hyundai based)
- Port fuel injected gaseous fuel
- Altronics CD-200 spark ignition system
- Full exhaust emission analysis capability
- Possibility of using NG or pure gaseous fuels

Number of cylinders	1
Number of intake/exhaust values	1/1
Bore [mm]	130
Stroke [mm]	140
Displacement [L]	1.85
Compression ratio	11:1
Fueling system	
Method	Fumigation, well-mixed
Natural Gas	Piped NG (~ 93% CH_4 v\v%)

Courtesy of A. Shah and M. Biruduganti, ANL

Pre-chamber Igniter with active fueling capability

- In-house, modular pre-chamber design for flexibility needed for fundamental studies
- Relatively simple to change PC volume, nozzle geometry, number, and orientation
- Close collaboration with SNL and NREL to achieve "common PC design"